Materials Computation Center, University of Illinois

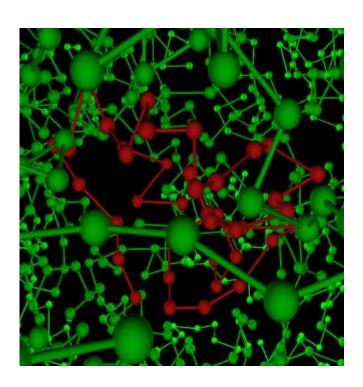
Duane Johnson and Richard Martin, NSF DMR-9976550

Polymer Shapes in Multicomponent Solutions
from co-PI: Erik Luijten

Research

Polymer chains in a solution typically coil up into a rather "random" object, which is commonly thought of as being spherical. In reality, however, polymer coils are rather aspherical, cigar-shaped objects. This "asphericity" directly influences the thermodynamic and flow properties of polymer solutions. Thus, we have used computer simulations to study how polymer shapes change in a solution containing several types of polymers. At certain temperatures and concentrations, such a solution exhibits phase separation. We found that phase separation leads to a radical change of the polymer shapes. We have quantified this shape variation for a variety of conditions.

Work done by graduate student L. Guo; see L. Guo and E. Luijten, Macromolecules **36**, 8201–8204 (2003).



After phase separation, each phase consists of a majority species (green in the figure) and a minority species (red). As can be clearly seen, the minority species coils up into a rather spherical object, "shying away" from the majority species.